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Aqua(5-bromidonicotinato)trimethyltin(IV)

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The Sn atom in the title complex, $[Sn(CH_3)_3(C_6H_3BrNO_2)(H_2O)]$, is five-coordinate with a distorted trigonal–bipyramidal geometry. The O atom of the carboxylate group occupies one of the axial sites and the O atom of the water molecule occupies the other. Water H atoms are involved in an intermolecular hydrogen-bonded network with the uncoordinated carboxylate O atom and the pyridine N atom.

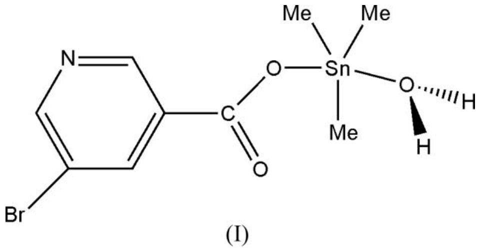
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
R factor = 0.024
wR factor = 0.062
Data-to-parameter ratio = 17.3

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

Organotin esters of carboxylic acids are widely used as biocides, as fungicides and, in industry, as homogeneous catalysts. Studies on organotin complexes containing carboxylate ligands with an additional donor atom (*e.g.* N, O or S) that is available for coordinating to the Sn atom have revealed that new structural types may lead to different activities. We have therefore synthesized the title compound, (I), and present its crystal structure here.



(I)

The molecular structure of (I) is shown in Fig. 1. The Sn atom assumes a trigonal–bipyramidal coordination geometry, formed by three methyl groups, a monodentate carboxylate group and a coordinated water molecule. The Sn1—O2 distance is 3.103 (3) Å, showing no significant interaction between the two atoms. In the crystal structure, the water O atoms are linked to adjacent carboxylate O atoms and adjacent N atoms of the pyridine ring *via* O—H···O and O—H···N hydrogen bonds, respectively (Table 2).

Experimental

The reaction was carried out under a nitrogen atmosphere. 5-Bromonicotinic acid (1 mmol) and sodium ethoxide (1.2 mmol) were added to benzene (30 ml) in a Schlenk flask and the mixture was stirred for 0.5 h. Trimethyltin(IV) chloride (1 mmol) was then added to the reactor and the reaction mixture was stirred for 12 h at 313 K. The resulting clear solution was evaporated under vacuum. The product was crystallized from a mixture of dichloromethane/methanol (1:1) (yield 80%, m.p. 430 K). Analysis calculated for $C_9H_{14}BrNO_3Sn$: C 28.24, H 3.69, N 3.66%; found: C 28.64, H 3.29, N 3.96%.

Crystal data

$[Sn(CH_3)_3(C_6H_3BrNO_2)(H_2O)]$
$M_r = 382.81$
Orthorhombic, *Pbca*
$a = 10.9478\ (18)$ Å
$b = 12.688\ (2)$ Å
$c = 19.479\ (3)$ Å
$V = 2705.7\ (8)$ Å^3
$Z = 8$
Mo *Kα* radiation
$\mu = 4.83$ mm^{-1}
$T = 298\ (2)$ K
0.38 × 0.27 × 0.21 mm

Data collection

Siemens SMART CCD area detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.261$, $T_{max} = 0.430$ (expected range = 0.220–0.363)
13116 measured reflections
2376 independent reflections
1902 reflections with $I > 2\sigma(I)$
$R_{int} = 0.060$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.024$
$wR(F^2) = 0.062$
$S = 1.07$
2376 reflections
137 parameters
H-atom parameters constrained
$\Delta\rho_{max} = 0.59$ e Å^{-3}
$\Delta\rho_{min} = -0.70$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Sn1—C8	2.099 (4)	Sn1—O1	2.187 (2)
Sn1—C9	2.112 (4)	Sn1—O3	2.412 (3)
Sn1—C7	2.113 (4)		
C8—Sn1—C9	124.59 (19)	C7—Sn1—O1	91.45 (14)
C8—Sn1—C7	117.78 (19)	C8—Sn1—O3	82.17 (13)
C9—Sn1—C7	116.08 (19)	C9—Sn1—O3	87.22 (16)
C8—Sn1—O1	96.13 (14)	C7—Sn1—O3	88.44 (14)
C9—Sn1—O1	94.61 (16)	O1—Sn1—O3	178.01 (11)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3···N1^{i}	0.85	2.01	2.849 (4)	168
O3—H1···O2^{ii}	0.85	1.84	2.684 (4)	169

Symmetry codes: (i) $x, -y+\frac{3}{2}, z+\frac{1}{2}$; (ii) $x-\frac{1}{2}, -y+\frac{3}{2}, -z+1$.

H atoms were positioned geometrically, with O—H = 0.85 Å and C—H = 0.93 and 0.96 Å for aromatic and methyl H atoms, respectively, and constrained to ride on their parent atoms, with $U_{iso}(H) = xU_{eq}(C,O)$ where $x = 1.5$ for methyl and aqua H and $x = 1.2$ for all other H atoms.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

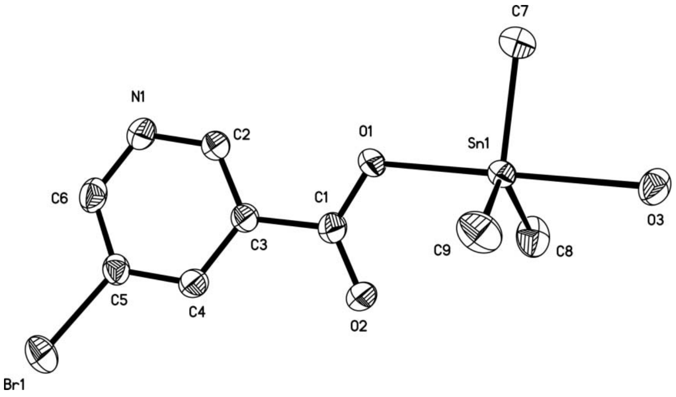


Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme. H atoms have been omitted for clarity.

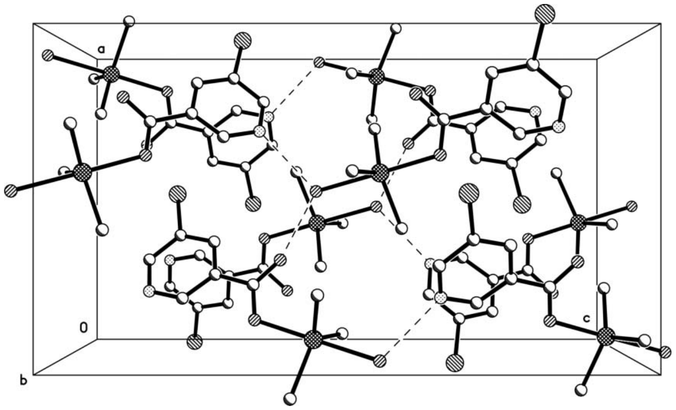


Figure 2
Crystal packing of (I). H atoms have been omitted for clarity. Hydrogen bonds are shown as dashed lines.

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Acta Cryst. (2007). E**63**, m1226–m1227 Wang *et al.* • $[Sn(CH_3)_3(C_6H_3BrNO_2)(H_2O)]$ **m1227**